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Phonon Spectrum in Hydroxyapatite: Calculations and EPR Study at Low Temperatures

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Abstract

© 2015 Springer Science+Business Media New York Density functional theory-based calculations within the framework of the plane-wave pseudopotential approach are carried out to define the phonon spectrum of hydroxyapatite (Formula presented.) (HAp). It allows to describe the temperature dependence of the electronic spin-lattice relaxation time (Formula presented.) of the radiation-induced stable radical (Formula presented.) in HAp, which was measured in X-band (9 GHz, magnetic field strength of 0.34 T) in the temperature range T = (10–300) K. It is shown that the temperature behavior of (Formula presented.) at (Formula presented.) 20 K can be fitted via two-phonon Raman type processes with the Debye temperature (Formula presented.) evaluated from the phonon spectrum.

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Keywords

Debye model, DFT, Phonons, Spin-lattice relaxation